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APPLICATION OF BEST LINEAR UNBIASED PREDICTION TO INTERPOLATION--ETC(U)
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APPLICATION OF BEST LINEAR UNBIASED
PREDICTION TO INTERPOLATION OF RANDOM
FIELDS AND TO NETWORK DESIGN.

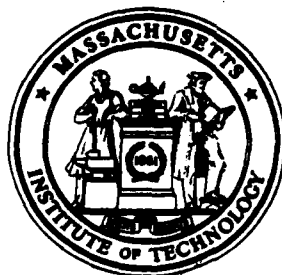
by

André Cabannes

DEPARTMENT OF MATHEMATICS
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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APPLICATION OF BEST LINEAR UNBIASED
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André Cabannes
Massachusetts Institute of Technology

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ABSTRACT

The practical problem of monitoring air pollutant concentration over a geographical area, or of estimating the mining resources in a region or a field can both be formulated as a problem of interpolation of random field.

Given a real-valued random field $\{Z(x), x \in \mathbb{R}^n\}$ the basic problem is to interpolate Z over an area A from measurements taken at n stations x_1, x_2, \dots, x_n , when the distribution of Z is only partially specified. The second problem is the choice of the network of stations. After deriving the form of the best linear unbiased predictor of Z we prove a general updating theorem which is useful both practically to quicken the computation of the new estimated map, and theoretically to study the problem of network design. Then we use this theorem to prove that when Z is a "smooth" random field (essentially differentiable in quadratic mean) the variance of estimation error of $Z(x)$ is a discontinuous function of the arguments x_1, x_2, \dots, x_n . We discuss the practical consequences of this result in the design of networks of stations.

Key words: Best linear unbiased predictor, random field, covariance function, differentiability in quadratic mean, network design.

1. Introduction and summary:

The practical problem of monitoring air pollutant concentration over a geographical area, or of estimating the mining resources in a region or a field can both be formulated as a problem of interpolation of a random field.

A random field is a real valued stochastic process $\{Z(x), x \in \mathbb{R}^m\}$ indexed in a multidimensional set, usually a two-dimensional spatial area. The problem considered here is to estimate $Z(x)$ for all $x \in A$ (some region of interest) from observations $Z(x_1), Z(x_2), \dots, Z(x_n)$ made at n points, and when the probability distribution of the random field is only partially specified. The points x_1, x_2, \dots, x_n are called the monitoring stations.

After having presented the model, which is akin to a linear regression model (mean function known up to a vector of parameters, covariance function known) and the method of estimation, in Section 2 we prove a useful updating theorem: if $\hat{Z}(x)$ is the estimator of $Z(x)$ based on $Z(x_1), Z(x_2), \dots, Z(x_n)$ and $\hat{Z}_y(x)$ that based on $Z(x_1), Z(x_2), \dots, Z(x_n)$ and $Z(y)$ we show that

$$\hat{Z}_y(x) = \hat{Z}(x) + \alpha[\hat{Z}(y) - Z(y)]$$

where α has a simple form.

Then in Section 3 we apply this theorem to the problem of

network design. It is shown that, contrary to a common belief, a network of stations $\{x_1, x_2, \dots, x_n\}$ where some stations are close to each other does not in general produce redundant information. Specifically

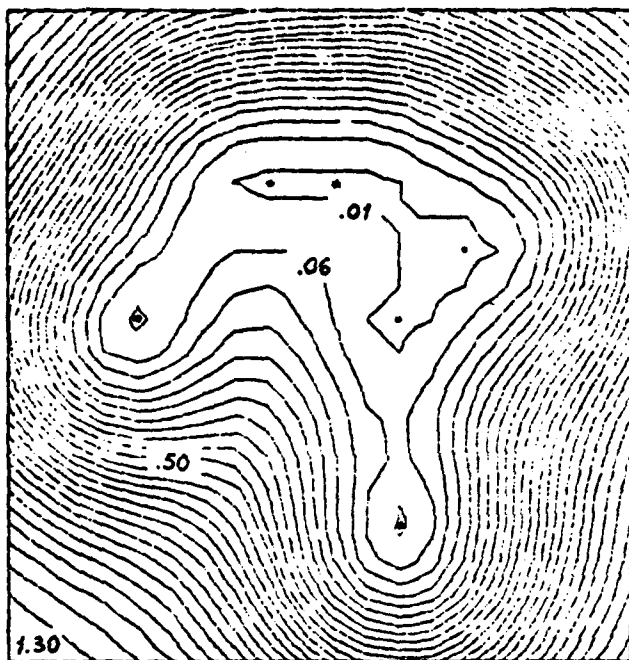
$$(1.1) \quad \lim_{y \rightarrow x_n} \text{Var}\{\hat{Z}_y(x) - Z(x)\} < \text{Var}\{\hat{Z}(x) - Z(x)\}$$

The most interesting condition under which (1.1) is true is when the covariance function (assumed isotropic) is of the form

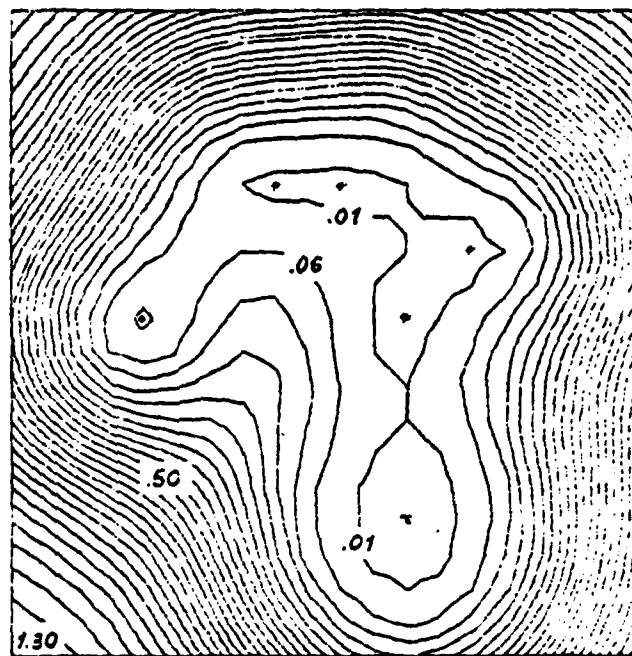
$$(1.2) \quad K(h) = \sigma^2 \left(1 - \frac{a^2}{2} h^2 + o(h^2)\right)$$

If the covariance function is only of the form $K(h) = \sigma^2(1 - ah + o(h))$ for $a > 0$, then equality holds in expression (1). Explicit formulas for $\lim_{y \rightarrow x_n} \text{Var}\{\hat{Z}_y(x) - Z(x)\}$ are given in each case.

A stationary random field whose covariance function is of the form (1.2) is differentiable in quadratic mean. As a consequence of the above result it is possible to improve the estimation, based on some network, of a smooth random field without "building" new stations (see figure below showing the variance of estimation of a stationary random field with covariance function $K(h) = e^{-\beta h^2}$).



1a



1b

Figure 1. Example of improvement of a network of six stations for estimation of a smooth random field. Figure 1a represents the level curves of the function $\text{Var}(\hat{Z}(x) - Z(x))$ in the standard use of the network; figure 1b shows the improvement realized by taking three measurements close to each other instead of one at a single station.

The method that we use to estimate (or "interpolate", or "predict") $Z(x)$ is the classical best linear unbiased prediction. A simple concise presentation of it is given by Goldberger (1962). This method has also been extensively applied, and given some new theoretical developments, by Matheron and his colleagues. They dubbed their whole body of techniques Kriging, see Delfiner (1975) and further references given there.

In another paper (Cabannes 1979 b) , meant to parallel the present one, the author shows some optimal statistical properties of best linear unbiased predictors.

2. The model; the best linear unbiased predictor; and an updating theorem:

Given the random field $\{Z(x), x \in \mathbb{R}^m\}$ we want to estimate $Z(x)$, at some fixed point x , from the observations $Z(x_1), Z(x_2), \dots, Z(x_n)$. To do that we assume the following model:

1) The random field has a covariance function $K(x,y) = \text{cov}(Z(x), Z(y))$ which is entirely specified. That is to say, in practice, it is known to us.

2) The mean function $m(x) = E Z(x)$ is only partially specified. We make the assumption that it is of the form

$$m(x) = a_1 f_1(x) + a_2 f_2(x) + \dots + a_p f_p(x)$$

where p and the functions $f_1(x), f_2(x), \dots, f_p(x)$ are known to

us, while the parameters a_1, a_2, \dots, a_p are unknown. The following examples will make this assumption clear:

a) assume that the mean function is an unknown constant m . This corresponds to $p = 1$, $f_1(x) \equiv 1$, $a_1 = m$.

b) in a two-dimensional random field $\{Z(x), x \in \mathbb{R}^2\}$ assume the mean function is an unknown plane. If we denote by $u(x)$ and $v(x)$ the components of the point x , this corresponds to $p = 3$, $f_1(x) \equiv 1$, $f_2(x) = u(x)$ and $f_3(x) \equiv v(x)$, while a_1, a_2, a_3 are the coefficients of the plane.

The method of estimation that we choose is the best linear unbiased prediction. That is, we will use the estimator $\hat{Z}(x)$ such that

- 1) $\hat{Z}(x) = \lambda_1(x)Z(x_1) + \lambda_2(x)Z(x_2) + \dots + \lambda_n(x)Z(x_n)$
- 2) $E \hat{Z}(x) = m(x)$ for all values of the parameters a_i 's.
- 3) $E\{\hat{Z}(x) - Z(x)\}^2$ is minimum.

Note: the third requirement is meaningful because an estimator satisfying conditions (1) and (2) is necessarily such that its mean squared error does not depend on the a_i 's.

We adopt the following condensed notation:

$$\underline{Z} = \begin{pmatrix} Z(x_1) \\ Z(x_2) \\ \vdots \\ Z(x_n) \end{pmatrix} = \text{the network observations}$$

K = covariance matrix of \underline{Z}

k_x = covariance vector between $Z(x)$ and \underline{Z}

$f_x = (f_1(x), f_2(x), \dots, f_p(x))'$

$a = (a_1, a_2, \dots, a_p)'$ so that $m(x) = f_x' a$

$$F' = \begin{bmatrix} f_1(x_1) & f_2(x_1) & \dots & f_p(x_1) \\ \vdots & \vdots & & \vdots \\ f_1(x_n) & f_2(x_n) & \dots & f_p(x_n) \end{bmatrix}$$

thus $E\underline{Z} = F'a$

$\lambda = (\lambda_1(x), \lambda_2(x), \dots, \lambda_n(x))'$

The calculations leading to the best linear unbiased predictor are classical (see Goldberger (1962), for instance). The optimal λ is

$$(2.1) \quad \lambda = K^{-1}k_x - K^{-1}F'(FK^{-1}F')^{-1}FK^{-1}k_x + K^{-1}F'(FK^{-1}F')^{-1}f_x$$

and the mean squared error using the B.L.U.E. is

$$(2.2) \quad \begin{aligned} \text{Var}(\hat{Z}(x) - Z(x)) &= K(x, x) - k_x' K^{-1} k_x \\ &\quad + (FK^{-1}k_x - f_x)' (FK^{-1}F')^{-1} (FK^{-1}k_x - f_x) \end{aligned}$$

To the above list we add the following notation:

$$G = FK^{-1}F'$$

$$\phi_x = FK^{-1}k_x - f_x$$

Goldberger made the observation that the B.L.U.E. of $Z(x)$ can be rewritten

$$\hat{Z}(x) = f_x' \hat{a} + k_x' K^{-1} [Z - F' \hat{a}]$$

where $\hat{a} = G^{-1}FK^{-1}Z$ is the generalized least square estimator of a using Z . For further explanations on the natural form of $\hat{Z}(x)$ see Cabannes (1979 a) .

Theorem 2.1: (Updating theorem)

Let $\hat{Z}_y(x)$ be the B.L.U.E. of $Z(x)$ based on the augmented set of observations $Z(x_1), Z(x_2), \dots, Z(x_n)$ and $Z(y)$. Then $\hat{Z}_y(x)$ and $\hat{Z}(x)$ (which is the B.L.U.E. based on Z) are related as follows:

$$(2.3) \quad \hat{Z}_y(x) = \hat{Z}(x) - \frac{\text{cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y))}{\text{Var}(\hat{Z}(y) - Z(y))} [\hat{Z}(y) - Z(y)]$$

and

$$(2.4) \quad \frac{\text{Var}(\hat{Z}_y(x) - Z(x))}{\text{Var}(\hat{Z}(x) - Z(x))} = 1 - \rho^2(x, y)$$

where $\rho(x, y) = \text{corr}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y))$

Proof: (*) Since $\hat{Z}_y(x)$ is a linear function of $Z(x_1), Z(x_2), \dots, Z(x_n), Z(y)$ while $\hat{Z}(x)$ and $\hat{Z}(y)$ are linear functions only of $Z(x_1), Z(x_2), \dots, Z(x_n)$, we can write

$$\begin{aligned}\hat{Z}_y(x) - \hat{Z}(x) &= \alpha[\hat{Z}(y) - Z(y)] + \beta_1 Z(x_1) + \beta_2 Z(x_2) + \dots + \beta_n Z(x_n) \\ &= \alpha[\hat{Z}(y) - Z(y)] + \beta' \underline{Z}\end{aligned}$$

where the coefficients α and $\beta_1, \beta_2, \dots, \beta_n$ depend on x_1, x_2, \dots, x_n, x and y .

The first objective is to show that $\beta' \underline{Z} = 0$. Since $E \hat{Z}_y(x) = E \hat{Z}(x)$ and $E \hat{Z}(y) = E Z(y)$, we deduce that $E \beta' \underline{Z} = 0$.

Next suppose that $\text{cov}(\hat{Z}(x) - Z(x), \beta' \underline{Z}) = c \neq 0$, then we can construct a linear unbiased estimator of $Z(x)$ which is better than the B.L.U.E. Indeed consider $\hat{Z}(x) + \gamma \beta' \underline{Z}$: it is linear, unbiased and

$$\begin{aligned}\text{Var}(\hat{Z}(x) + \gamma \beta' \underline{Z} - Z(x)) &= \\ \text{Var}(\hat{Z}(x) - Z(x)) + 2\gamma c + \gamma^2 \text{Var} \beta' \underline{Z}\end{aligned}$$

hence the choice $\gamma = -\frac{c}{\text{Var} \beta' \underline{Z}}$ makes

$\text{Var}(\hat{Z}(x) + \gamma \beta' \underline{Z} - Z(x)) < \text{Var}(\hat{Z}(x) - Z(x))$. This is a contradiction. Therefore $\beta' \underline{Z}$ is uncorrelated with $\hat{Z}(x) - Z(x)$.

(*) I am grateful to Yi-Ching Yao for this proof which simplifies my original one using partitioned matrices.

The same argument shows that $\beta' \underline{Z}$ is uncorrelated with $\hat{Z}(x) - Z(x)$, and also with $\hat{Z}(y) - Z(y)$. From this it is easy to conclude that $\text{Var } \beta' \underline{Z} = 0$. This is done as follows:

note that $\beta' \underline{Z} = \hat{Z}_y(x) - \hat{Z}(x) - \alpha[\hat{Z}(y) - Z(y)] = \hat{Z}_y(x) - Z(x) - [\hat{Z}(x) - Z(x)] - \alpha[\hat{Z}(y) - Z(y)]$; hence, from $\text{Var } \beta' \underline{Z} = \text{cov}(\beta' \underline{Z}, \beta' \underline{Z})$, substituting the above expression for one of the $\beta' \underline{Z}$, we get $\text{Var } \beta' \underline{Z} = 0$. From this we conclude that $\beta' \underline{Z} = 0$.

It remains to show that the coefficient α has the form given in formula (2.3). Since $\beta' \underline{Z} = 0$ we can write

$$\hat{Z}_y(x) - Z(x) - [\hat{Z}(x) - Z(x)] = \alpha[\hat{Z}(y) - Z(y)]$$

take on both sides the covariance with $\hat{Z}(y) - Z(y)$, and note that, for the same reasons as above, $\hat{Z}_y(x) - Z(x)$ is uncorrelated with $\hat{Z}(y) - Z(y)$. This yields $-\text{cov}(\hat{Z}(y) - Z(y), \hat{Z}(x) - Z(x)) = \alpha \text{Var}(\hat{Z}(y) - Z(y))$ and establishes formula (2.3).

To prove formula (2.4) write

$$\hat{Z}_y(x) - Z(x) = \hat{Z}(x) - Z(x) + \alpha[\hat{Z}(y) - Z(y)]$$

and take variances on both sides. This gives

$$\begin{aligned} \text{Var}(\hat{Z}_y(x) - Z(x)) &= \text{Var}(\hat{Z}(x) - Z(x)) \\ &\quad + \alpha^2 \text{Var}(\hat{Z}(y) - Z(y)) \\ &\quad + 2\alpha \text{cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y)) \end{aligned}$$

and using the expression obtained for α we get

$$\text{Var}(\hat{Z}_y(x) - Z(x)) = \text{Var}(\hat{Z}(x) - Z(x)) [1 - c^2(x,y)] \quad \text{where} \\ c^2(x,y) = \text{corr}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y))$$

Q.E.D.

This updating theorem is very useful to compute the new estimated map $\{\hat{Z}_y(x), x \in A\}$ from the already computed values $\{\hat{Z}(x), x \in A\}$. We refer the reader to Cabannes (1979a) for details and an illustration of this point. The theorem is also useful to study theoretically the problem of network design.

In Section 3, to apply theorem 2.1 it is convenient to have for the coefficient α a more explicit form. We already have the explicit expression

$$\text{Var}(\hat{Z}(y) - Z(y)) = K(y,y) - k_y' K^{-1} k_y + \phi_y' G^{-1} \phi_y$$

given (slightly differently) by formula (2.2). The next theorem gives an analogous expression for the covariance term in the coefficient α :

Theorem 2.2

$$(2.5) \quad \text{Cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y)) = K(x,y) - k_x' K^{-1} k_y + \phi_x' G^{-1} \phi_y :$$

proof: From formula (2.1) for the vector of coefficients λ in $\hat{Z}(x)$ we can write

$$\hat{Z}(x) = k_x' K^{-1} \underline{Z} - \phi_x' G^{-1} F K^{-1} \underline{Z}$$

then $\text{cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y))$

$$\begin{aligned} &= \text{cov}(\hat{Z}(x), \hat{Z}(y)) - \text{cov}(Z(x), \hat{Z}(y)) \\ &\quad - \text{cov}(\hat{Z}(x), Z(y)) + \text{cov}(Z(x), Z(y)) \\ &= (k_x' K^{-1} - \phi_x' G^{-1} F K^{-1}) K (K^{-1} k_y - K^{-1} F' G^{-1} \phi_y) \\ &\quad - \lambda'(y) k_x - \lambda'(x) k_y + K(x, y) \end{aligned}$$

after developing and cancelling terms in this expression we obtain formula (2.5)

Q.E.D.

3. Application to study of continuity of $\text{Var}(\hat{Z}(x) - Z(x))$ and to network design:

In this section we apply theorem 2.1 to the study of what happens when two or more monitoring stations of the network are close to each other. And we show that interesting results occur when the random field Z is smooth in a stochastic sense.

In order to be able to state results with simple formulas we will specialize to an isotropic covariance function: the function $K(x, y)$ will only depend on $\|y - x\|$.

The hinge of the next theorem is that an isotropic random field $\{Z(x), x \in \mathbb{R}^m\}$ is differentiable in quadratic mean if and only if its covariance function is of the form

$K(x,y) = \sigma^2 \left(1 - \frac{a^2}{2} \|x-y\|^2 + o(\|x-y\|^2) \right)$. This result still holds if Z has a differentiable non constant mean function and an isotropic covariance function.

For convenience we introduce the following notation:

$s(x; x_1, x_2, \dots, x_n) = \text{Var}(\hat{Z}(x) - Z(x))$ where $\hat{Z}(x)$ is based on the network x_1, x_2, \dots, x_n . Consequently, according to the definition in Section 2,

$$s(x; x_1, x_2, \dots, x_n, y) = \text{Var}(\hat{Z}_y(x) - Z(x))$$

Theorem 3.1: If a random field $\{Z(x), x \in \mathbb{R}^m\}$, with differentiable mean function and isotropic covariance function, is differentiable in quadratic mean, then the function $s(x; x_1, x_2, \dots, x_n, y)$ is not continuous in y , in the sense that

$$\lim_{y \rightarrow x_n} s(x; x_1, x_2, \dots, x_n, y) \neq s(x; x_1, x_2, \dots, x_n).$$

Indeed, we have

$$(3.1) \quad \lim_{y \rightarrow x_n} \frac{s(x; x_1, x_2, \dots, x_n, y)}{s(x; x_1, x_2, \dots, x_n)} = 1 - \rho^*{}^2$$

(with fixed direction)

with

$$(3.2) \quad \rho^* = \kappa \frac{w'(x_n - y)}{[(x_n - y)' A (x_n - y)]^{1/2}}$$

where κ is a constant, w is a vector, and A is a positive definite quadratic form, each depending only on x, x_1, x_2, \dots, x_n .

In the case $n = 1$, formula (3.2) simplifies to

$$(3.3) \quad \rho^* = \kappa \cos(\widehat{y x_n x})$$

where $\widehat{y x_n x}$ is the angle between the directions of $y - x_n$ and $x - x_n$.

If the random field is not differentiable but continuous in quadratic mean and $K(h) = \sigma^2(1 - ah + o(h))$, $a > 0$, then $s(x; x_1, x_2, \dots, x_n, y)$ is continuous in y in the sense indicated above.

Finally, if the random field is not continuous in q.m., then again the function $s(x; x_1, x_2, \dots, x_n, y)$ is not continuous in y .

Proof. If the random field, with differentiable mean function and isotropic covariance function, is differentiable then

$$K(x, y) = \sigma^2(1 - \frac{a^2}{2} \|x - y\|^2 + o(\|x - y\|^2)) .$$

With no loss of generality, let's take $\sigma = 1$.

In theorem 2.1 we proved that

$$(3.4) \quad \frac{s(x; x_1, x_2, \dots, x_n, y)}{s(x; x_1, x_2, \dots, x_n)} = 1 - \rho^2(x, y)$$

where

$$(3.5) \quad \rho(x, y) = \frac{\text{cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y))}{[\text{Var}(\hat{Z}(x) - Z(x)) \text{Var}(\hat{Z}(y) - Z(y))]}^{1/2},$$

\hat{Z} being computed on the basis of x_1, x_2, \dots, x_n . To prove theorem 3.1 we shall derive the expansion of $\rho(x, y)$, when $y \rightarrow x_n$, by computing those of

$$(3.6) \quad \text{Var}(\hat{Z}(y) - Z(y)) = 1 - k_y' K^{-1} k_y + \phi_y' G^{-1} \phi_y$$

and

$$(3.7) \quad \text{Cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y)) = K(x, y) - k_x' K^{-1} k_y + \phi_x' G^{-1} \phi_y.$$

We need a Taylor expansion of $K(x, y)$ when $y \rightarrow x_n$. To do this it will be convenient to use for $K(x, y)$ the form

$$(3.8) \quad K(x, y) = R\left(\frac{a^2}{2} \|x - y\|^2\right)$$

So we have $R(t) = 1 - t + o(t)$ as $t \rightarrow 0$. Next note that

$$(3.9) \quad \|x - y\|^2 = \|x - x_n\|^2 + 2(x - x_n)'(x_n - y) + \|x_n - y\|^2,$$

hence

$$\begin{aligned} R\left(\frac{a^2}{2} \|x - y\|^2\right) &= R\left(\frac{a^2}{2} \|x - x_n\|^2\right) + \\ &\quad \frac{a^2}{2} [2(x - x_n)'(x_n - y) + \|x_n - y\|^2] R^{[1]}\left(\frac{a^2}{2} \|x - x_n\|^2\right) + \\ &\quad o(\|x_n - y\|), \end{aligned}$$

$(R^{[1]})$ denotes the first derivative of the function R). From (3.8) we conclude that for all x

$$(3.10) \quad K(x, y) = K(x, x_n) + a^2 (x - x_n)' (x_n - y) R^{[1]} \left(\frac{a^2}{2} \|x - x_n\|^2 \right) + o(\|x_n - y\|),$$

while for x_n

$$(3.11) \quad K(x_n, y) = 1 - \frac{a^2}{2} \|x_n - y\|^2 + o(\|x_n - y\|^2).$$

First we apply (3.10) and (3.11) to

$$k_y = \begin{pmatrix} K(x_1, y) \\ \vdots \\ K(x_{n-1}, y) \\ K(x_n, y) \end{pmatrix}.$$

With the following notation

$$(3.12) \quad \Omega = a^2 \begin{bmatrix} (x_1 - x_n)' R^{[1]} \left(\frac{a^2}{2} \|x_1 - x_n\|^2 \right) \\ \vdots \\ (x_{n-1} - x_n)' R^{[1]} \left(\frac{a^2}{2} \|x_{n-1} - x_n\|^2 \right) \\ -\frac{1}{2} (x_n - y)' \end{bmatrix}$$

and

$$(3.13) \quad \varepsilon = \begin{pmatrix} o(\|x_n - y\|) \\ \vdots \\ o(\|x_n - y\|) \\ o(\|x_n - y\|^2) \end{pmatrix}$$

we can write

$$(3.14) \quad k_y = k_{x_n} + \Omega(x_n - y) + \varepsilon$$

Secondly, applying (3.14) to $\phi_y = FK^{-1}k_y - f_y$ we obtain

$$\begin{aligned} \phi_y &= FK^{-1}k_{x_n} + FK^{-1}\Omega(x_n - y) + FK^{-1}\varepsilon - f_y \\ &= f_{x_n} + FK^{-1}\Omega(x_n - y) + FK^{-1}\varepsilon - f_y \\ (3.15) \quad &= (FK^{-1}\Omega + f_{x_n}^{[1]})(x_n - y) + \eta \end{aligned}$$

where $f_{x_n}^{[1]} = [\text{grad } f_y]_{y=x_n}$, and η is a p-dimensional vector, each component of which is $o(\|x_n - y\|)$.

With these preliminaries, now we can compute the variance and covariance given in (3.6) and (3.7). Using (3.14) and (3.15) we obtain, on the first hand,

$$\begin{aligned} \text{Var}(\hat{Z}(y) - Z(y)) &= 1 - (k_{x_n} + \Omega(x_n - y) + \varepsilon)' K^{-1} (k_{x_n} + \Omega(x_n - y) + \varepsilon) \\ (3.16) \quad &+ [(FK^{-1}\Omega + f_{x_n}^{[1]})(x_n - y) + \eta]' G^{-1} [(FK^{-1}\Omega + f_{x_n}^{[1]})(x_n - y) + \eta]. \end{aligned}$$

Since $k_{x_n}' K^{-1} k_{x_n} = 1$, $k_{x_n}' K^{-1} \Omega = -\frac{a^2}{2} (x_n - y)'$ and $k_{x_n}' K^{-1} \varepsilon = o(\|x_n - y\|^2)$, the R.H.S. of (3.16) becomes

$$\begin{aligned} &a^2 \|x_n - y\|^2 - (x_n - y)' \Omega' K^{-1} \Omega (x_n - y) + o(\|x_n - y\|^2) + \\ (3.17) \quad &(x_n - y)' [FK^{-1}\Omega + f_{x_n}^{[1]}]' G^{-1} [FK^{-1}\Omega + f_{x_n}^{[1]}] (x_n - y) + o(\|x_n - y\|^2) \end{aligned}$$

or in condensed notation

$$(3.18) \quad (x_n - y)' A (x_n - y) + o(\|x_n - y\|^2) ,$$

where A (which depends only on x_1, x_2, \dots, x_n and x) is a positive definite quadratic form since (3.18) is the expansion of a variance. On the other hand, we have

$$(3.19) \quad \begin{aligned} \text{Cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y)) &= K(x, y) - k'_x K^{-1} (k_{x_n} + \Omega(x_n - y) + \varepsilon) + \\ &\quad \phi'_x G^{-1} (F K^{-1} \Omega + f_{x_n}^1) (x_n - y) + \eta . \end{aligned}$$

Using (3.10) and $k'_x K^{-1} k_{x_n} = K(x, x_n)$, the R.H.S. of (3.19) simplifies to

$$(3.20) \quad \begin{aligned} &a^2 (x - x_n)' (x_n - y) R^{[1]} \left(\frac{a^2}{2} \|x - x_n\|^2 \right) + o(\|x_n - y\|) - \\ &k'_x K^{-1} \Omega (x_n - y) - k'_x K^{-1} \varepsilon + \end{aligned}$$

$$\phi'_x G^{-1} [F K^{-1} \Omega + f_{x_n}^{[1]}] (x_n - y) + \phi'_x G^{-1} \eta$$

or in condensed notation

$$(3.21) \quad w' (x_n - y) + o(\|x_n - y\|) .$$

where w is a vector depending only on x_1, x_2, \dots, x_n and x .

Now substituting (3.18) and (3.21) in formula (3.5) we obtain

$$(3.22) \quad \rho(x, y) = \frac{w'(x_n - y) + o(\|x_n - y\|)}{\{\text{Var}(\hat{Z}(x) - Z(x)) [(x_n - y)' A(x_n - y) + o(\|x_n - y\|^2)]\}^{1/2}}$$

The first part of the theorem, i.e., formula (3.2), follows from (3.22) when we let y tend to x_n .

In the case $n = 1$, to establish the more explicit formula (3.3), we must go back to formulas (3.17) and (3.20). Observe that in this case

$$a) \quad \Omega = -a^2(x_n - y)'$$

$$b) \quad F = 1 \quad \text{and} \quad f_{x_n}^{[1]} = 0.$$

$$c) \quad K, G, K^{-1}, \text{ and } G^{-1} \text{ are equal to } 1,$$

hence (3.17) becomes

$$(3.23) \quad \text{Var}(\hat{Z}(y) - Z(y)) = a^2 \|x_n - y\|^2 + o(\|x_n - y\|^2)$$

and (3.20) becomes

$$(3.24) \quad \text{Cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y)) =$$

$$a^2 (x - x_n)' (x_n - y) R^{[1]} \left(\frac{a^2}{2} \|x - x_n\|^2 \right) + o(\|x_n - y\|).$$

Since we have

$$[a^2 \|x_n - y\|^2 + o(\|x_n - y\|^2)]^{1/2} = a \|x_n - y\| + o(\|x_n - y\|) ,$$

from (3.23) and (3.24), we conclude that

$$\rho(x, y) = \kappa \frac{(x - x_n)'(y - x_n)}{\|x - x_n\| \|y - x_n\|} + o(\|x_n - y\|) ,$$

where κ is a scalar independent of y . This completes the proof of formula (3.3)

Some more calculations, that we omit, show that in the case $n = 1$ the constant κ is actually equal to

$$\frac{a \|x - x_n\| R^{[1]}(\frac{a^2}{2} \|x - x_n\|^2)}{[2(1 - R(\frac{a^2}{2} \|x - x_n\|^2))]^{1/2}} = \frac{d}{du} [(1 - R(u^2))^{1/2}] ,$$

where

$$u = \frac{a}{\sqrt{2}} \|x - x_n\| .$$

We now consider the case when the random field is not differentiable but continuous in q.m. and $K(h) = 1 - ah + o(h)$, with $a > 0$. To establish the continuity of $s(x; x_1, x_2, \dots, x_n, y)$ we use the same scheme as before. The important difference is that $\|x - y\|$ plays the role of $\|x - y\|^2$ and formula (3.9) is replaced by

$$\begin{aligned}
 \|x-y\| &= [\|x-x_n\|^2 + 2(x-x_n)'(x_n-y) + \|x_n-y\|^2]^{1/2} \\
 &= \|x-x_n\| \left[1 + \frac{2(x-x_n)'(x_n-y)}{\|x-x_n\|^2} + \frac{\|x_n-y\|^2}{\|x-x_n\|^2} \right]^{1/2} \\
 &= \|x-x_n\| \left[1 + \frac{(x-x_n)'(x_n-y)}{\|x-x_n\|^2} + o(\|x_n-y\|) \right] \\
 &= \|x-x_n\| + \frac{(x-x_n)'(x_n-y)}{\|x-x_n\|} + o(\|x_n-y\|) .
 \end{aligned}$$

Formulas (3.10) and (3.11) become the following: For all x

$$(3.26) \quad K(x,y) = K(x,x_n) + a \frac{(x-x_n)'(x_n-y)}{\|x-x_n\|} R^{[1]}(a\|x-x_n\|) + o(\|x_n-y\|)$$

while for x_n

$$K(x_n,y) = 1 - a\|x_n-y\| + o(\|x_n-y\|) .$$

To express k_y we use the new notation

$$(3.28) \quad \Omega_1 = \begin{bmatrix} (x_1-x_n)' \frac{R^{[1]}(a\|x_1-x_n\|)}{\|x_1-x_n\|} \\ \vdots \\ (x_{n-1}-x_n)' \frac{R^{[1]}(a\|x_{n-1}-x_n\|)}{\|x_{n-1}-x_n\|} \\ - \frac{(x_n-y)'}{\|x_n-y\|} \end{bmatrix}$$

and

$$\varepsilon_1 = \begin{pmatrix} o(\|x_n - y\|) \\ \vdots \\ o(\|x_n - y\|) \\ o(\|x_n - y\|) \end{pmatrix}$$

The difference between ε given by (3.13) and ε_1 given by (3.29) is that the last component of ε_1 is $o(\|x_n - y\|)$ instead of being $o(\|x_n - y\|^2)$.

Formulas (3.14) and (3.15) still hold with Ω_1 and ε_1 substituting for Ω and ε . But the calculations made in (3.16), (3.17), and (3.18) are replaced by

$$(3.30) \quad \text{Var}(\hat{Z}(y) - Z(y)) = a\|x_n - y\| + o(\|x_n - y\|).$$

On the other hand, formula (3.21), giving the development of $\text{Cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y))$ is still true. Therefore

$$\text{Cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y)) = o(\|x_n - y\|),$$

whereas, from (3.30)

$$[\text{Var}(\hat{Z}(y) - Z(y))]^{1/2} = o(\|x_n - y\|^{1/2}).$$

We conclude that

$$\lim_{\|y-x_n\| \rightarrow 0} \rho(x,y) = 0 ,$$

and this, in view of (3.4), establishes the continuity of $s(x; x_1, x_2, \dots, x_n, y)$.

Lastly, when the random field is not continuous in quadratic mean, the covariance function $K(h)$ is not continuous at the origin. Then neither $\text{Cov}(\hat{Z}(x) - Z(x), \hat{Z}(y) - Z(y))$ nor $\text{Var}(\hat{Z}(y) - Z(y))$ tend to zero when $\|y-x_n\|$ tends to zero. Hence $\rho(x,y) \not\rightarrow 0$ and s is not continuous. Q.E.D.

We now conclude this section with a discussion of the interpretation of the theorem just proved, and a discussion of the consequences for network design. Consider for simplicity a two-dimensional random field $\{Z(x), x \in \mathbb{R}^2\}$.

Before interpreting the theorem just proved, we observe that expressions (3.17) and (3.20) are often well approximated by expressions (3.23) and (3.24). As a consequence, the formula

$$\rho^* = \kappa \cos(\widehat{y x_n x})$$

is an approximation, even when $n > 1$, to the more complicated formula (3.2) which enters expression (3.1), giving the reduction of uncertainty at x when a station y is added in the vicinity of x_n .

The interpretation of Theorem 3.1 is that when station y is very close to x_n three possibilities can arise:

1. $K(h)$ has a jump at the origin and Z can be decomposed

into two parts

$$Z = \zeta + \varepsilon ,$$

where ζ is a random field with isotropic covariance function continuous at the origin, and ε is an independent stationary white noise. Then the couple $\{Z(y), Z(x_n)\}$ provides information on the variance of ε that $Z(x_n)$ alone does not provide.

2. $K(h) = 1 - ah + o(h)$, Z is continuous in q.m. but not differentiable. Then $Z(y)$ and $Z(x_n)$, in the limit, measure the same thing and do not provide more information than $Z(x_n)$ alone.

3. However, if $K(h) = 1 - \frac{a^2}{2} h^2 + o(h^2)$, Z is differentiable, and then $\{Z(y), Z(x_n)\}$ provides information on the partial derivative of Z at x_n in the direction of $y - x_n$. In the case $n = 1$ the reduction of uncertainty about $Z(x)$ at any x is proportional to the square of the cosine of the angle between $y - x_1$ and $x - x_1$.

The three cases considered above do not exhaust the possible forms of isotropic covariance functions in \mathbb{R}^2 . However, the cases left over are pathological cases such as, for instance, a function $K(h)$ for which

$$\limsup_{h \rightarrow 0} K(h) \neq \liminf_{h \rightarrow 0} K(h)$$

or, an isotropic covariance function continuous but not differentiable at the origin. Such covariance functions are not used in practice.

The preceding interpretation can be given the following extension, that we have not proved: When the random field Z is

differentiable in quadratic mean, three measurements $\{Z(x_n), Z(y_1), Z(y_2)\}$, where y_1 and y_2 are very close to x_n , and the directions of $y_1 - x_n$ and $y_2 - x_n$ are different, for instance perpendicular, will provide all possible information on the first-order partial derivatives of Z at x_n . They will determine the tangent plane. Moreover, in the limit the reduction of uncertainty on $Z(x)$ at any point x will be independent of the directions $y_1 - x_n, y_2 - x_n$, provided they are not the same. We can give the following non rigorous justification for this fact: when y_1 and y_2 are very close to x_n the data $\{Z(x_1), Z(x_2), \dots, Z(x_n), Z(y_1), Z(y_2)\}$ is equivalent to $\{Z(x_1), Z(x_2), \dots, Z(x_n), Z'_{y_1}(x_n), Z'_{y_2}(x_n)\}$. Moreover, if z_1 and z_2 are two other points close to x_n , $Z'_{y_1}(x_n)$ and $Z'_{y_2}(x_n)$ are related to $(Z'_{z_1}(x_n), Z'_{z_2}(x_n))$ by a linear relationship; therefore the data are also equivalent to $\{Z(x_1), Z(x_2), \dots, Z(x_n), Z'_{z_1}(x_n), Z'_{z_2}(x_n)\}$, and finally to $\{Z(x_1), Z(x_2), \dots, Z(x_n), Z(z_1), Z(z_2)\}$.

In the design of networks used to monitor smooth random phenomena like, for instance, barometric pressure, or variation of temperature over an area in high altitude, or used to estimate smooth geological random fields, the discontinuity of $s(x; x_1, x_2, \dots, x_n, y)$ and of its average $t(x_1, x_2, \dots, x_n, y) = \int_A s(x; x_1, x_2, \dots, x_n, y) dx$ when $y \rightarrow x_n$ is of practical interest.

If we want to improve an existing network in a given area the first idea, if we are to use the criterion t , is to find the point y in A minimizing $t(x_1, x_2, \dots, x_n, y)$ and build a new station or take a new measurement there.

However, we can generally do better in terms of the same criterion by taking, at each already existing stations, three measurements close to each other and forming an angle. This would require only some minor modification in the routine of taking measurements at stations, and would altogether cost much less money than to build a new station.

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